I claim:

1.   A method for determining the movement of particles,
particularly impurities, in a medium, under the influence of a
changing interface between two neighboring phases, comprising
the steps of
(a) Determining the temporal and/or local evolution of said interfac
(b) Determining the movement of said particles in dependence
of the temporal and/or local evolution of the phase interface
as determined in step (a).

2.   A method according to claim 1, comprising the further step
of
(c) determining the distribution of the particles at a certain
time.

3.   A method according to claim 1, comprising the further step
of determining the distribution of the particles at a steady
state position of the phase interface.

4.   A method according to claim 1, wherein the method is
performed on the basis of a model defining the medium as
having a phase interface described as a smooth transition over
a non zero range of the medium.

5.   A method according to claim 1, wherein the method is
performed on the basis of a model defining the medium as
having a phase interface which is described by a discontinuous
transition between the two phases.

6.   A method according to claim 4, wherein the method
performed on the basis of a model wherein the medium is
described by a data field having a first value for the first

phase and a second value for the second phase and values in between representing the smooth transition.

7. A method according to claim 6, wherein the evolution of said data field is calculated by a differential equation.

8. A method according to claim 6, wherein the method is applied for a medium of a material having at least one crystalline phase and where the data field is describing the crystallinity or a related parameter.

9. A method according to claim 8, wherein the determination of step (a) is determined by a differential equation of the form

$$\frac{dC}{dt} = div(\alpha \cdot grad(C)) + \beta \cdot C \cdot (1-C) \cdot (C-\gamma) \ .$$

wherein C is the data field of the crystallinity or a related parameter of the material, div and grad are spatial differential operators and α, β and γ are parameters which determine the environmental conditions of the simulation.

10. A method according to claim 5, wherein the evolution of the phase interface is determined by the calculation of probabilities for regions adjacent to the phase interface to switch from one phase into the other in a certain time period, using a monte carlo type random algorithm.

11. A method according to claim 1, wherein said movement of the particles is calculated by a monte carlo type simulation of discrete particle hopping, where the hopping probability of a particle depends on the potential energy of the initial and the final particle position of the hopping event, and where the potential energy of the particle depends on the material

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phase.

12. A method according to claim 5, wherein the evolution of the phase interface is calculated by means of a movement function of the discontinuity between the phases.

13. A method according to claim 1, wherein the evolution of the phase interface or the movement and/or the distribution of the particles is calculated in dependence of a high temperature treatment of the medium.

14. A method according to claim 1, wherein the evolution of the phase interface and/or the movement of the particles is calculated in dependence of a potential difference between the two phases.

15. A method according to claim 1, wherein the evolution of the phase interface is calculated in dependence of the concentration of the particles.

16. A method according to claim 1, wherein said movement of particles is calculated in dependence of a driving force induced by the difference of potential energy in the two phases.

17. A method according to claim 5, wherein the movement of the particles at the discontinuous transition between the two phases is determined in dependence of an accumulation of particles at said transition and a particle transport which is proportional to the number of accumulated particles and to the velocity of the discontinuous transition between the two phases.

18. A method according to claim 1, wherein the method is performed for a medium made of a semiconductor material and having at least two different phases and the particles being dopants of the semiconductor.

19. A method according to claim 18, wherein the method is performed for a semiconductor having at least one crystalline and one amorphous phase and a phase interface in between.

20. A method according to claim 19, wherein the method is applied for at least one of the following processes:
- dopant redistribution during SPE regrowth
- Indium dopant loss
- Arsenic dopant loss
- Fluorine dose loss
- Arsenic dopant activation during SPE regrowth
- Boron uphill diffusion during SPE regrowth

21. A method according to claim 18, wherein the method is performed for a semiconductor having at least one solid and one liquid phase and a phase interface in between.

22. A method according to claim 21, wherein the method is applied on dopant redistribution during LPE regrowth.

23. A method according to claim 22, wherein the method is applied on dopant redistribution during float zone purification processes.

24. A method according to claim 18, wherein the method is applied for the dopant redistribution during LASER annealing processes where the laser is powerful enough to melt or amorphize an illuminated region of the semiconductor material.

25. A computer program product comprising software code portions for performing a method according to claim 1 when run on a computer.